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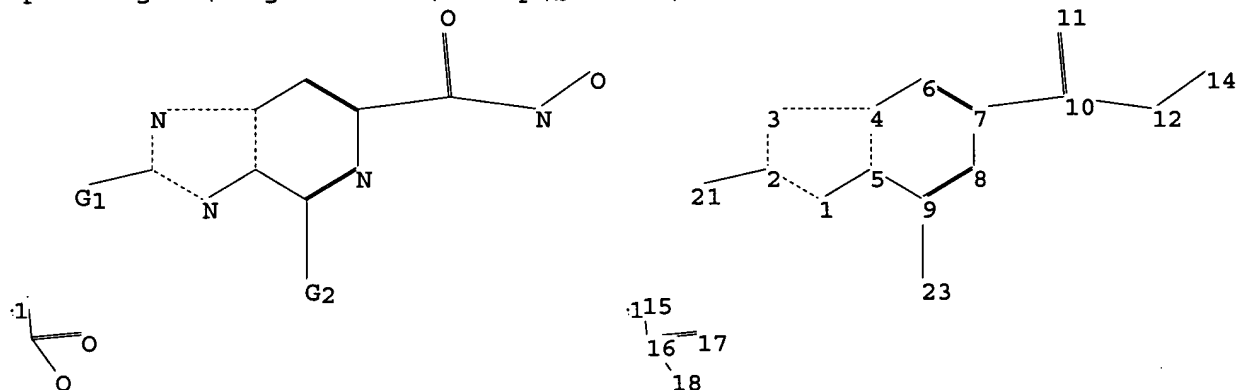
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10-699068.str



chain nodes :

11 14 15 16 17 18 21 23

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

10 12

chain bonds :

2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18

ring bonds :

1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9

exact/norm bonds :

1-2 1-5 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14 16-17 16-18

exact bonds :

7-10 15-16

isolated ring systems :

containing 1 :

G1:H, [*1]

G2:H,Ak

Match level :

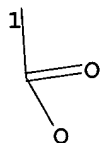
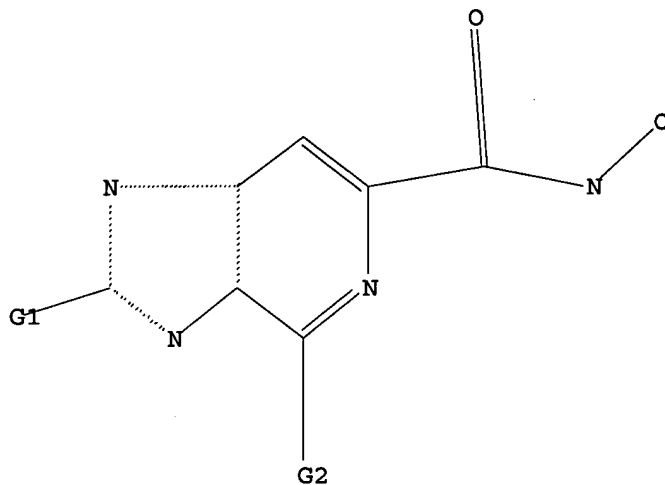
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS
23:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1 H, [O1]

G2 H, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful

FULL SEARCH INITIATED 06:10:34 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1220 TO ITERATE

100.0% PROCESSED 1220 ITERATIONS

SEARCH TIME: 00.00.01

21 ANSWERS

L2 21 SEA SSS FUL L1

=> fil caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

166.94

167.15

FILE 'CAPLUS' ENTERED AT 06:10:38 ON 28 APR 2006

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 28 Apr 2006 VOL 144 ISS 18
FILE LAST UPDATED: 26 Apr 2006 (20060426/ED)

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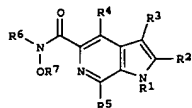
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L3 2 L2

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L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:1171056 CAPLUS
 DN 143:440391
 TI Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase.
 IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewe, Michael Bruno; Tanis, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang, Junhu
 PA Pfizer Inc., USA
 SO PCT Int. Appl., 177 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 PAN CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005103003	A2	20051103	WO 2005-IB1029	20050414
WO 2005103003	A3	20060316		
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AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HK, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RN: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KD, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005277662	A1	20051215	US 2004-565705P	P 20040426
			US 2005-660502P	P 20050309
			US 2005-115003	20050425
			US 2004-565705P	P 20040426
			US 2005-660502P	P 20050309

OS MARPAT 143:440391
 GI



AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9)NR10R11, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6 = H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 (substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3), were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in DMF for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μM in an HIV-1 cell protection assay.

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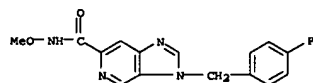
L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
IT 688314-07-0P 868550-24-7P 868550-25-8P

868550-26-9P 868550-27-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase)

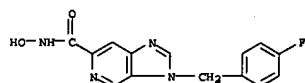
RN 688314-07-0 CAPLUS

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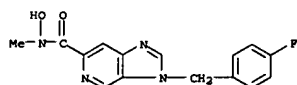
RN 868550-24-7 CAPLUS

CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)



RN 868550-25-8 CAPLUS

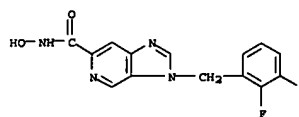
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(4-fluorophenyl)methyl]-N-hydroxy-N-methyl- (9CI) (CA INDEX NAME)



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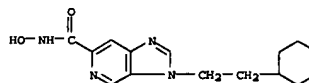
CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-[(2,3-difluorophenyl)methyl]-N-hydroxy- (9CI) (CA INDEX NAME)

L3 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 868550-27-0 CAPLUS

CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-hydroxy- (9CI) (CA INDEX NAME)

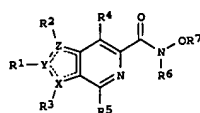


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L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:390246 CAPLUS
 DN 140:406796
 TI Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors
 IN Hu, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu
 PA Pfizer Inc., USA
 SO PCT Int. Appl., 108 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 PAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004039803	A2	20040513	WO 2003-1B4735	20031027
WO 2004039803	A3	20040916		
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RM: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KQ, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2500487	AA	20040513	US 2002-2500487	20031027
			US 2002-422513P	P 20021031
			WO 2003-1B4735	W 20031027
AU 2003269421	A1	20040525	AU 2003-269421	20031027
			US 2002-422513P	P 20021031
			WO 2003-1B4735	W 20031027
EP 1558611	A2	20050803	EP 2003-751203	20031027
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, ES, HU, SK				
BR 2003015820	A	20050913	US 2002-422513P	P 20021031
			WO 2003-1B4735	W 20031027
JP 2006506398	T2	20060223	JP 2004-547905	20031027
			US 2002-422513P	P 20021031
			WO 2003-1B4735	W 20031027
US 2004147547	A1	20040729	US 2002-422513P	P 20021031
NL 1024676	A1	20040506	NL 2003-1024676	20031031
NL 1024676	C2	20051214	US 2002-422513P	P 20021031
OS MARPAT 140:406796				
GI				

L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



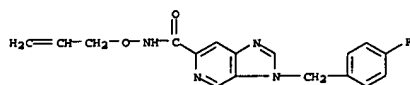
AB Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc = halo, H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, alkynyl, heteroalkyl, (hetero)cycloalkyl, or (hetero)aryl; X = C or N; Y = C or N; Z = C or N; or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof] were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions, such as AIDS (no data). Examples include 31 synthetic prepn. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addnl. prepn. of bicyclic hydroxamates without data, bioassays for HIV-integrase activity and HIV-1 cell protection without data. For instance, Et 1H-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NaH in DMF to give the N-alkylated pyrrolopyridinecarboxylate (48%). Saponification with NaOH in MeOH provided the acid (55%), which was treated with HONH2·HCl in the presence of HATU and TEA to afford (2,4-difluorobenzyl)-N-hydroxy-1H-pyrrolo[2,3-c]pyridine-5-carboxamide (II) in 48% yield.

IT 688313-86-2P, 3-((2,4-Difluorobenzyl)-N-hydroxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 688313-90-8P, 1-((2,4-Difluorobenzyl)-N-hydroxy-1H-imidazo[4,5-c]pyridine-6-carboxamide 688314-02-5P, N-Benzyl-3-((4-fluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-07-0P, 3-((4-Fluorobenzyl)-N-methoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-08-1P, 3-((4-Fluorobenzyl)-N-phenoxyl-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-09-2P, 3-((4-Fluorobenzyl)-N-((2,3,4,5,6-pentafluorobenzyl)oxy)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-10-5P, N-(Allyloxy)-3-((4-

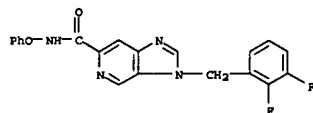
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 fluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-23-0P

3-((2,3-Difluorobenzyl)-N-phenoxyl-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-24-1P, 3-((2,3-Difluorobenzyl)-N-methoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-25-2P, N-Allyloxy-3-((2,3-difluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-26-3P, 1-((4-Fluorobenzyl)-N-phenoxyl-1H-imidazo[4,5-c]pyridine-6-carboxamide 688314-27-4P, N-tert-Butoxy-3-((2,3-difluorobenzyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-28-5P, N-Methoxy-3-((3-methylbutyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-29-6P, 3-((3-Methylbutyl)-N-phenoxyl-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-30-9P, 3-((2-Cyclohexylethyl)-N-phenoxyl-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-31-0P, 3-((2-Cyclohexylethyl)-N-methoxy-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-32-1P, N-Allyloxy-3-((2-cyclohexylethyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-33-2P, N-Allyloxy-3-((2-cyclohexylethyl)-3H-imidazo[4,5-c]pyridine-6-carboxamide 688314-34-3P, 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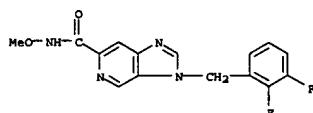
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



RN 688314-23-0 CAPLUS
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
 3-[(2,3-difluorophenyl)methyl]-N-
 phenoxy- (9CI) (CA INDEX NAME)

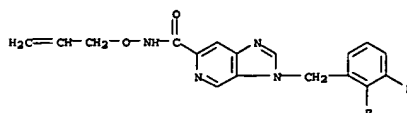


RN 688314-24-1 CAPLUS
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
 3-[(2,3-difluorophenyl)methyl]-N-
 methoxy- (9CI) (CA INDEX NAME)

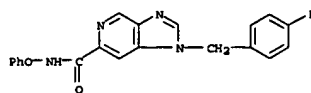


RN 688314-25-2 CAPLUS
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
 3-[(2,3-difluorophenyl)methyl]-N-
 (2-propenyloxy)- (9CI) (CA INDEX NAME)

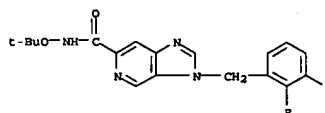
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



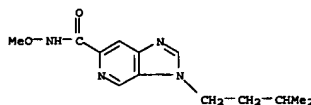
RN 688314-26-3 CAPLUS
 CN 1H-Imidazo[4,5-c]pyridine-6-carboxamide, 1-[(4-fluorophenyl)methyl]-N-
 phenoxy- (9CI) (CA INDEX NAME)



RN 688314-27-4 CAPLUS
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide,
 3-[(2,3-difluorophenyl)methyl]-N-
 (1,1-dimethylethoxy)- (9CI) (CA INDEX NAME)

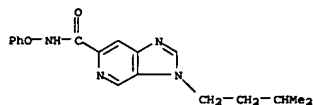


RN 688314-28-5 CAPLUS
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, N-methoxy-3-(3-methylbutyl)-
 (9CI) (CA INDEX NAME)

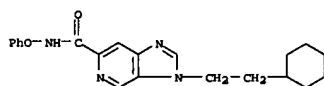


RN 688314-29-6 CAPLUS

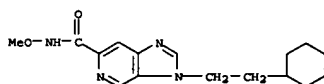
L3 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(3-methylbutyl)-N-phenoxymethyl-
 (9CI) (CA INDEX NAME)



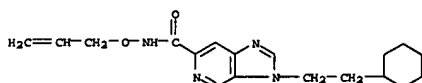
RN 688314-30-9 CAPLUS
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-phenoxymethyl-
 (9CI) (CA INDEX NAME)



RN 688314-31-0 CAPLUS
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 (9CI) (CA INDEX NAME)

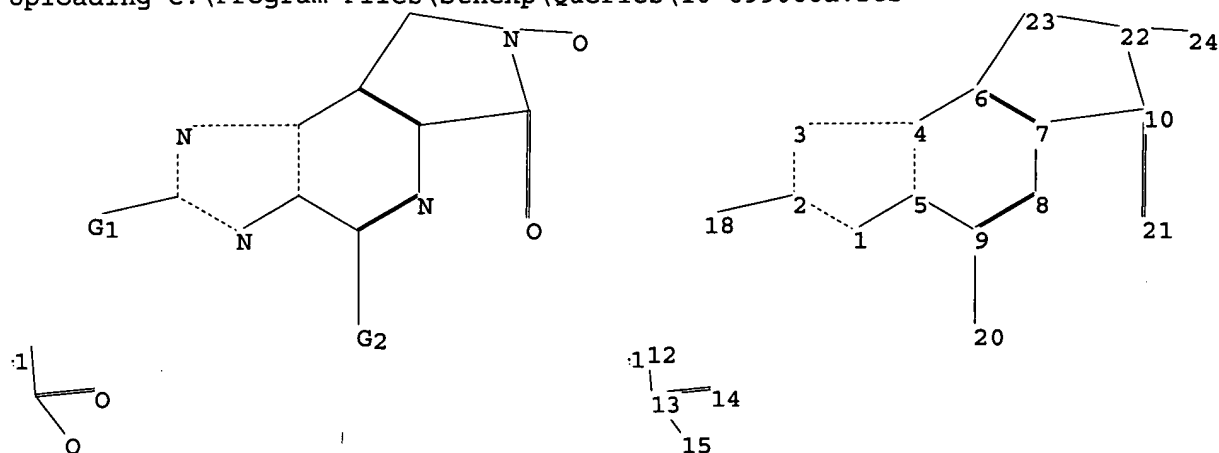


RN 688314-32-1 CAPLUS
 CN 3H-Imidazo[4,5-c]pyridine-6-carboxamide, 3-(2-cyclohexylethyl)-N-(2-
 propenyloxy)- (9CI) (CA INDEX NAME)



=>

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chain nodes :

12 13 14 15 18 20 21 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 22 23

chain bonds :

2-18 9-20 10-21 12-13 13-14 13-15 22-24

ring bonds :

1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 6-23 7-8 7-10 8-9 10-22 22-23

exact/norm bonds :

1-2 1-5 2-3 2-18 3-4 4-6 4-5 5-9 6-7 6-23 7-8 7-10 8-9 9-20 10-21

10-22 13-14 13-15 22-23 22-24

exact bonds :

12-13

isolated ring systems :

containing 1 :

G1:H, [*1]

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

12:CLASS 13:CLASS 14:CLASS 15:CLASS 18:CLASS 20:CLASS 21:CLASS 22:Atom

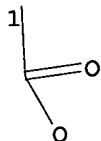
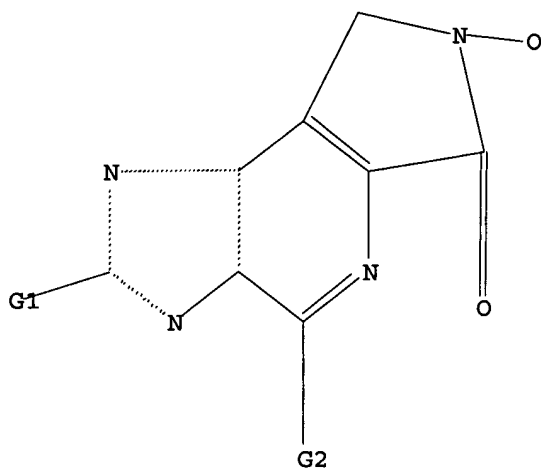
23:Atom 24:CLASS

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



G1 H, [1]

G2 H, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 14 ful

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 06:13:51 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 35 TO ITERATE

100.0% PROCESSED 35 ITERATIONS
SEARCH TIME: 00.00.01

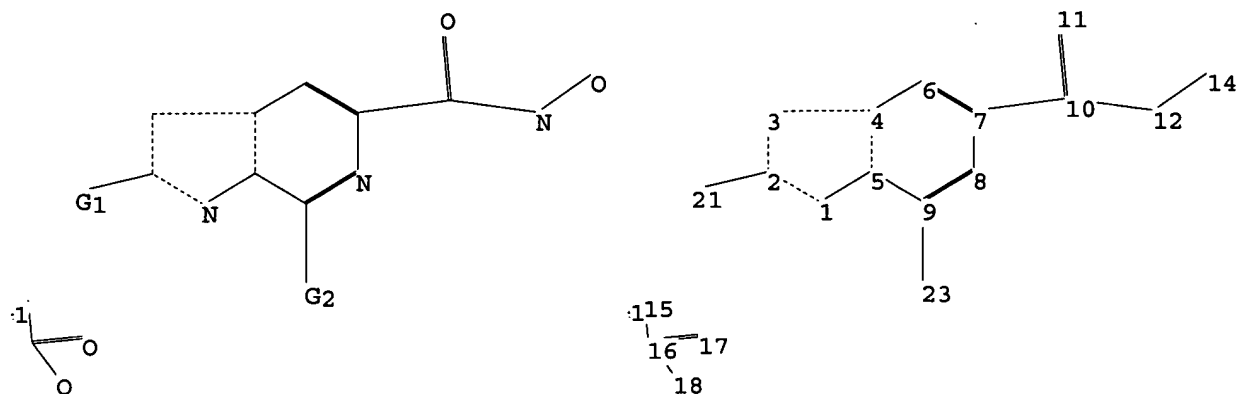
0 ANSWERS

L5 0 SEA SSS FUL L4

L6 0 L5

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Uploading C:\Program Files\Stnexp\Queries\10-699068b.str



chain nodes :

11 14 15 16 17 18 21 23

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

10 12

chain bonds :

2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18

ring bonds :

1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9

exact/norm bonds :

1-2 1-5 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14
16-17 16-18

exact bonds :

7-10 15-16

isolated ring systems :

containing 1 :

G1:H, [*1]

G2:H, Ak

Match level :

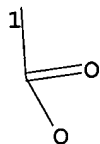
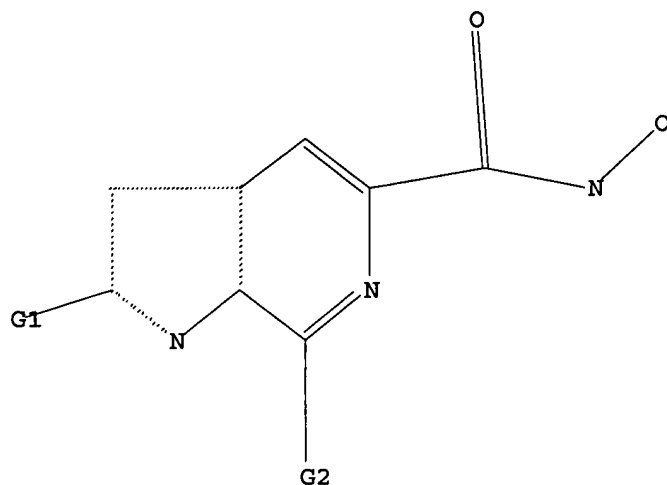
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS
23:CLASS

L7 STRUCTURE UPLOADED

=> d

L7 HAS NO ANSWERS

L7 STR



G1 H, [a1]

G2 H, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s 17 ful

REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 06:15:25 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1216 TO ITERATE

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100.0% PROCESSED      1216 ITERATIONS
SEARCH TIME: 00.00.02
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202 ANSWERS

L8 202 SEA SSS FUL L7

L9 4 L8

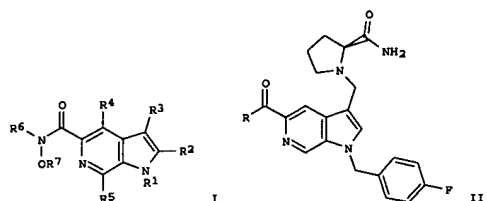
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L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2006:237568 CAPLUS
 DN 144:312070
 TI Preparation of N-hydroxy pyrrolopyridinecarboxamides as inhibitors of HIV integrase.
 IN Dress, Klaus; Kuehler, Jon Edward; Plewe, Michael Bruno; Yang, Anle;
 Zhang, Junhu
 PA Pfizer Inc., USA
 SO PCT Int. Appl., 99 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 PAN CNT 1

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 yield. The invented compds. are useful for the treatment of diseases mediated by HIV, such as AIDS and AIDS related complex.
 RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006027694	A1	20060316	WO 2005-182967	20050826
W: AB, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HD, IL, IN, IS, JP, KE, KG, KH, KP, KR, KZ, LC, LK, LA, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RM: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
			US 2004-607791P	P 20040907

GI



AB Title compds. I (wherein R1, R6 = H, (substituted) alkyl, alkenyl, etc.; R2, R5 = H; R3 = pyrrolidinylmethyl, piperidinylmethyl, etc.; R4 = H, halo, alkyl, etc.; R7 = H, heteroalkyl, aryl, etc.) and pharmaceutically acceptable salts and solvates thereof were prepared as inhibitors of HIV integrase. For instance, condensation of Me ester II (R = OMe) with hydroxylamine at ambient temperature gave hydroxyamide II (R = NHOR) in

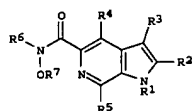
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L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:1371056 CAPLUS
 DN 143:440391
 TI Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase.
 IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Flewe, Michael Bruno; Tanis, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang, Junhu
 PA Pfizer Inc., USA
 SO PCT Int. Appl., 177 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2005103003	A2	20051103	WO 2005-IB1029	20050414
WO 2005103003	A3	20060316		
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RW:	BW, GH, GM, KE, LS, MM, MY, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, EG, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2005277662	A1	20051215	US 2004-565705P	P 20040426
			US 2005-660502P	P 20050309
			US 2005-115003	20050425
			US 2004-565705P	P 20040426
			US 2005-660502P	P 20050309

OS MARPAT 143:440391
 GI



AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9)CNR10R11, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6 = H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N

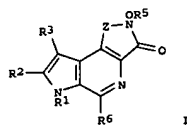
L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 (substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3), were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in DMP for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μM in an HIV-1 cell protection assay.

=> d fbib abs 3

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:1170952 CAPLUS
 DN 143:440390
 TI Preparation of pyrrolonaphthyridinones, pyranopyrrolopyridinones, and
 pyrrolopyridoazepinones as inhibitors of HIV integrase.
 IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewa, Michael
 Bruno; Tanis, Steven Paul; Zhu, Huichun; Zhang, Junhu
 PA Pfizer Inc., USA
 SO PCT Int. Appl., 90 pp.
 DT Patent
 LA English
 PAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005103051	A1	20051103	WO 2005-1B976	20050413
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MM, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CG, CI, CM, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2005277661	A1	20051215	US 2004-565728P	P 20040426
			US 2005-643316P	P 20050111
			US 2005-657594P	P 20050228
			US 2005-660430P	P 20050309
			US 2005-114813	20050425
			US 2004-565728P	P 20040426
			US 2005-643316P	P 20050111
			US 2005-657594P	P 20050228
			US 2005-660430P	P 20050309

OS MARPAT 143:440390
 GI



AB Title compds. [I: R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2 = H, alkyl; R3 = H, alkyl, (substituted) heteroalkyl, aminoalkyl, aminocarbonyl, etc.; Z = [C(R4)2]n, CR4:CR4, etc.; R4 = H, halo,

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 heteroalkyl, (substituted) alkyl, cycloalkyl, aryl, heteroalkyl, cycloheteroalkyl; R5 = H, heteroalkyl, aryl, alkenyl, (substituted) alkyl; R6 = H; n = 1-4), were prepd. Thus, 3-(4-fluorobenzyl)-7-hydroxy-3,7-dihydro-6H-pyrrolo[2,3-c]-1,7-naphthyridin-6-one (multistep prepn. given) showed EC50 = 0.4 nM in an HIV-1 cell protection assay.
 RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

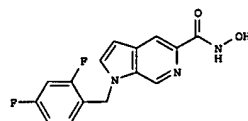
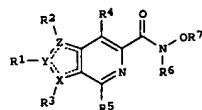
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L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2004:390246 CAPLUS
 DN 140:406796
 TI Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors
 IN Hu, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewa, Michael Bruno; Wang, Hai; Zhang, Junhu
 PA Pfizer Inc., USA
 SO PCT Int. Appl., 108 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN: CMT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004039803	A2	20040513	WO 2003-IB4735	20031027
WO 2004039803	A3	20040916		
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CA 2500487	AA	20040513	CA 2003-2500487	20031027
			US 2002-422513P	P 20021031
			WO 2003-IB4735	W 20031027
AU 2003269421	A1	20040525	AU 2003-269421	20031027
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			WO 2003-IB4735	W 20031027
EP 1558611	A2	20050803	EP 2003-751203	20031027
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BR 2003015820	A	20050913	US 2002-422513P	P 20021031
			WO 2003-IB4735	W 20031027
JP 2006506398	T2	20060223	JP 2004-547905	20031027
			US 2002-422513P	P 20021031
			WO 2003-IB4735	W 20031027
US 2004147547	A1	20040729	US 2003-699068	20031030
			US 2002-422513P	P 20021031
NL 1024676	A1	20040506	NL 2003-1024676	20031031
NL 1024676	C2	20051214		
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OS MARPAT 140:406796
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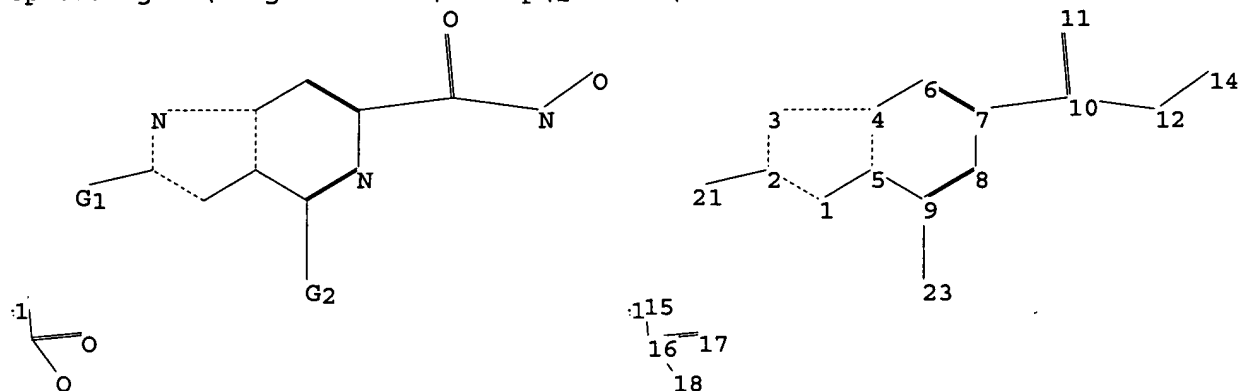
L9 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc = halo, H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, alkynyl, heteroalkyl, (hetero)cycloalkyl, or (hetero)aryl; X = C or N; Y = C or N; Z = C or N; or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof] were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions, such as AIDS (no data). Examples include 31 synthetic preps. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addnl. preps. of bicyclic hydroxamates without data, bioassays for HIV-integrase activity and HIV-1 cell protection without data. For instance, Et 1H-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NaH in DMF to give the N-alkylated pyrrolopyridinecarboxylate (48%). Saponification with NaOH in MeOH provided the acid (55%), which was treated with HONH2·HCl in the presence of HATU and TEA to afford (2,4-difluorobenzyl)-N-hydroxy-1H-pyrrolo[2,3-c]pyridine-5-carboxamide (II) in 48% yield.

=>

Uploading C:\Program Files\Stnexp\Queries\10-699068c.str



chain nodes :

11 14 15 16 17 18 21 23

ring nodes :

1 2 3 4 5 6 7 8 9

ring/chain nodes :

10 12

chain bonds :

2-21 7-10 9-23 10-11 10-12 12-14 15-16 16-17 16-18

ring bonds :

1-2 1-5 2-3 3-4 4-6 4-5 5-9 6-7 7-8 8-9

exact/norm bonds :

1-2 2-3 2-21 3-4 4-6 4-5 5-9 6-7 7-8 8-9 9-23 10-11 10-12 12-14 16-17 16-18

exact bonds :

1-5 7-10 15-16

isolated ring systems :

containing 1 :

G1:H, [*1]

G2:H,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:CLASS 12:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 21:CLASS

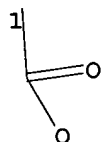
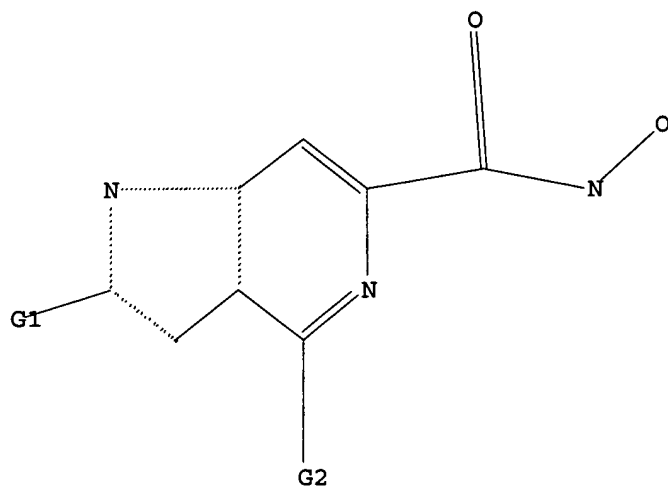
23:CLASS

L10 STRUCTURE UPLOADED

=> d

L10 HAS NO ANSWERS

L10 STR



G1 H, [01]

G2 H, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l10 ful

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 06:19:09 FILE 'REGISTRY'

SCREENING

SCREENING

FULL SCREEN SEARCH COMPLETED - 1028 TO ITERATE

100.0% PROCESSED 1028 ITERATIONS

12 ANSWERS

SEARCH TIME: 00.00.31

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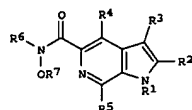
L12 2 L11

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L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
 AN 2005:1171056 CAPLUS
 DN 143:440391
 TI Preparation of N-hydroxy pyrrolopyrimidinecarboxamides as inhibitors of HIV integrase.
 IN Dress, Klaus Ruprecht; Hu, Qiyue; Johnson, Ted William; Plewa, Michael Bruno; Tanis, Steven Paul; Wang, Hai; Yang, Anle; Yin, Chunfeng; Zhang, Junhu
 PA Pfizer Inc., USA
 SO PCT Int. Appl., 177 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005103003	A2	20051103	WO 2005-1B1029	20050414
WO 2005103003	A3	20060316		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, GU, HK, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
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			US 2005-660502P	P 20050309
			US 2005-115003	20050425
			US 2004-565705P	P 20040426
			US 2005-660502P	P 20050309

OS MARPAT 143:440391
 GI



AB Title compds. [I; R1 = H, (substituted) alkyl, alkenyl, heteroalkyl; R2, R5 = H; R3 = (CR8R9)tNR10R11, (substituted) heteroalkyl; R4 = H, halo, alkyl, heteroalkyl, (substituted) alkenyl, alkynyl, OR12a, NR12aR12b; R6 = H, alkyl, heteroalkyl, (substituted) alkenyl; R8, R9 = H, alkyl; R10R11N

L12 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
 (substituted) cycloheteroalkyl; R12a, R12b, R12c = H, alkyl; t = 1-3], were prepd. Thus, 1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxylic acid (prepn. given) was stirred with O-(7-azabenzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate, Et3N, and NH2OH.HCl in DMF for 16 h to give 48% N-hydroxy-1-(2,4-difluorobenzyl)-1H-pyrrolo[2,3-c]pyridine-5-carboxamide. The latter showed an EC50 = 0.00795 μM in an HIV-1 cell protection assay.

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L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:390246 CAPLUS

DN 140:406796

TI Preparation of pyrrolo[2,3-c]pyridine hydroxamates as HIV-integrase inhibitors

IN Hu, Qiyue; Kuki, Atsuo; Nowlin, Dawn Marie; Plewe, Michael Bruno; Wang, Hai; Zhang, Junhu

PA Pfizer Inc., USA

SO PCT Int. Appl., 108 pp.

CODEN: PIXXD2

DT Patent

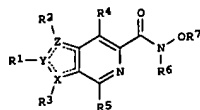
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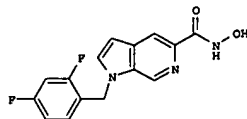
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004039803	A2	20040513	WO 2003-1B4735	20031027
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W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CP, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
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R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
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			US 2002-422513P	P 20021031

OS MARPAT 140:406796
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L12 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



I



II

AB Title bicyclic hydroxamate compds. I [wherein R1-R3 = independently H, CO2Rc, or (un)substituted (halo)alkyl, alkenyl, or heteroalkyl; Rc = halo,

H, OH, alkyl, alkenyl, alkynyl, (hetero)cycloalkyl, or (un)substituted (hetero)aryl; R4 and R6 = independently H or (un)substituted (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; R5 = H, (halo)alkyl, alkenyl, alkynyl, or heteroalkyl; or R4 and R6 together with the N to which R6 is attached may form a fused heterocycle; R7 = H or (un)substituted (halo)alkyl, alkenyl, alkynyl, heteroalkyl, (hetero)cycloalkyl, or (hetero)aryl; X = C or N; Y = C or N; Z = C or N; or a pharmaceutically acceptable salt, prodrug, or active metabolite thereof] were prepared as HIV-integrase inhibitors for the treatment of HIV-mediated diseases and conditions, such

as AIDS (no data). Examples include 31 synthetic preps. of pyrrolo[2,3-c]pyridine hydroxamates with data, 32 addnl. preps. of bicyclic hydroxamates without data, bioassays for HIV-integrase activity and HIV-1 cell protection without data. For instance, Et 1H-pyrrolo[2,3-c]pyridine-5-carboxylate was coupled with 2,4-difluorobenzyl bromide using NaH in DMF to give the N-alkylated pyrrolopyridinecarboxylate (48%). Saponification with NaOH in MeOH provided the acid (55%), which was treated with HONH2·HCl in the presence of HATU and TEA to afford (2,4-difluorobenzyl)-N-hydroxy-1H-pyrrolo[2,3-c]pyridine-5-carboxamide (II) in 48% yield.